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Title: Developing HE Simulants for Proton Radiography Experiments

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Developing HE Simulants for Proton Radiography Experiments

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Introduction

Over the past decade, proton radiography (pRad) has proved to be an increasingly useful tool in the study of high explosives (HE) science, such as investigating equation of state (EOS) models, material failure studies, and shock physics. Proton radiography is a unique tool for verification and validation of the hydrodynamics codes. At LANSCE, this is accomplished by conducting dynamic experiments that involve explosives such as PBX-9501 or PBX-9502. An inert material that could accurately simulate the radiographic properties of HE and replace it for calibration measurements would be very valuable.

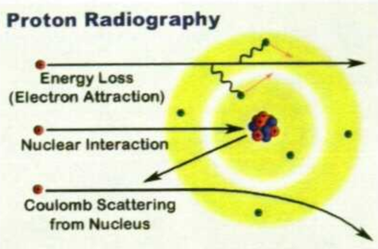


Fig. 1. There are three effects of interest that occur as protons pass through an object. These are Multiple Coulomb Scattering (MCS), energy loss (dE/dx), and nuclear interactions.

In a radiograph, MCS and nuclear interactions are factors in the proton transmission (N/N_o), while energy loss results in variations of proton momentum that cause blurring from chromatic aberrations.

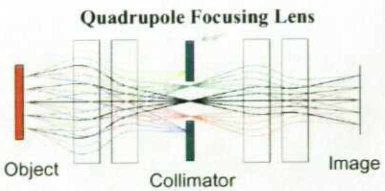


Fig. 2. Large scattering angles are stopped by the collimator. At the image plane, the transmitted protons are converted into light by a scintillating fiber optic array and captured by CCD readout cameras.

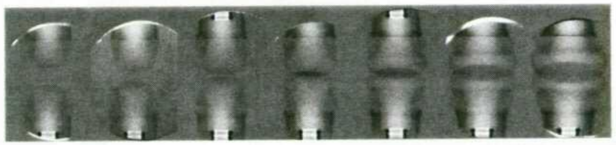


Fig. 3. Radiographs from a wave-collider experiment. Dynamic experiments such as this will benefit from an HE simulant for use in analysis an calibration.

Advantages of proton over x-ray radiography

- •Longer interaction length better suited for hydrotests
- •High detection efficiency of charged particles
- •Ability to transport and focus charged beam
- •Multi-pulse capability

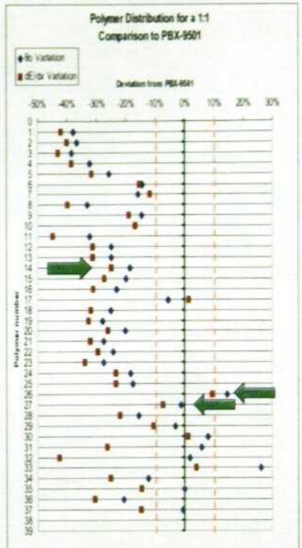
Materials and Methods

PBX-9501 and PBX-9502, like most explosives, are almost purely CHNO compounds with high percentages of nitrogen and oxygen. However, many potential substitute chemicals with similar chemical formulas are either flammable or explosive themselves, present health hazards, or are uncommon. To avoid these problems, we investigated polymers.

Most polymers are long chains of hydrocarbons that contain a high percentage of carbon, but some contain oxygen, nitrogen, halogens and other elements.

#	Polymer	Trade Name	Density (g/cm³)	Repeating Unit
1	Low Density Polyethylene	LDPE	0.92	C_2H_4
2	High Density Polyethylene	HDPE	0.96	C_2H_4
3	Polypropylene	PP	0.903	C_3H_6
4	Polystyrene	HIPS	1.06	C_8H_8
5	Polyacrylic Nitrile	PAN	1.2	C_3H_3N
6	Melamine formaldehyde	MF	1.5	$C_4H_6N_6$
7	Hexamethylenetetramine	Hexa	1.5	$C_6H_{12}N_4$
8	Acrylonitrile-Butadiene-Styrene	ABS	1.025	$C_{15}H_{17}N$
9	Polyoxymethylene (homopolymer)	POM	1.42	CH_2O
10	Polyoxymethylene (copolymer)	POM	1.41	CH_2O
11	Polyvinyl acetate		0.96	$C_4H_6O_2$
12	Polyethyl acrylate	PEA	1.18	$C_5H_8O_2$
13	Polymethyl methacrylate (Lucite)	PMMA/IM	1.18	$C_5H_8O_2$
14	Polyethylene terephthalate	PET	1.38	$C_{10}H_8O_4$
15	Cellulose acetate	CA	1.28	$C_{12}H_{16}O_8$
16	Cellulose acetate butyrate	CAB	1.2	$C_{15}H_{22}O_8$
17	Diallyl orthophthalate	DAP	1.8	$C_{14}H_{14}O_4$
18	Polycarbonates	PC	1.2	$C_{16}H_{14}O_3$
19	Nylon-6		1.13	$C_6H_{11}NO$
20	Urea formaldehyde	UF	1.3	$C_3H_6N_2O_2$
21	Nylon-66		1.14	$C_{12}H_{22}N_2O_2$
22	Polyurethane	Pellon U	1.2	$C_{17}H_{16}N_2O_4$
23	Nylon 6-T		1.14	$C_{14}H_{18}N_2O_2$
24	Poly p-Benzamide	Kevlar 49	1.38	$C_{14}H_{10}N_2O_2$
25	Polyimide	PI	1.4	$C_{22}H_{10}N_2O_5$
26	Polytetrafluoroethylene (Teflon)	PTFE	2.2	C_2F_4
27	Poly(vinylidene fluoride) (Kynar)	PVDF	1.76	$C_2H_2F_2$
28	Polyvinyl fluoride	Tedlar	1.4	C_2H_3F
29	Ethylene-tetrafluoroethylene	ETFE	1.7	$C_4H_4F_4$
30	Vinylidene fluoride-Hexafluoropropylene	Fluorel/Viton	2.0	$C_5H_2F_8$
31	Polyvinyl chloride	PVC	1.4	C_2H_3Cl
32	Chlorinated polyethylene	CPE	1.16	$C_2H_3Cl_2$
33	Polychlorotrifluoroethylene	PCTFE/Kel-F	2.13	C_2ClF_3
34	Polyethersulfone	PES	1.37	$C_{12}H_8O_3S$
35	Poly(phenylene sulfide)	PPS	1.57	C_6H_4S
36	Polysulfone	PSO	1.24	$C_{27}H_{22}O_4S$

Table 1. Name and properties of the polymers that were modeled. Hazardous polymers are shown in red.



Plot 1. We found the fluorine and chlorine containing polymers to be the closest match to the properties of PBX-9501 and PBX-9502.

Equations for pRad

Multiple Coulomb Scattering:

$$\theta_o = \frac{13.6\ MeV}{\beta c p} z \sqrt{\frac{x}{X_o}}\left[1+0.038\cdot\ln\left(\frac{x}{X_o}\right)\right]$$

Energy Loss:

$$-\frac{dE}{dx} = Kz^2\frac{Z}{A}\frac{1}{\beta^2}\left[\frac{1}{2}\cdot\ln\left(\frac{2m_ec^2\beta^2\gamma^2T_{max}}{I^2}\right)-\beta^2\right]$$

Transmission:

$$\frac{N}{N_o}=\left[1-\exp\left(\frac{-\theta^2}{2\theta_o^2}\right)\right]\cdot\exp\left(\frac{-x}{\lambda}\right)$$

Polymer benefits

- •Readily available
- •Inexpensive
- •Safe (nonreactive)
- •Easily machined and handled
- •Range of formulas and densities

Data and Results

A "step wedge" is used for pRad calibration to determine the range of areal densities seen in the dynamic object being radiographed. As a quality assurance measure, we validated our calculation models using previous radiographs.

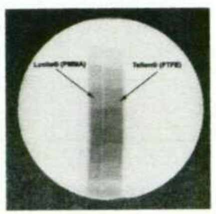
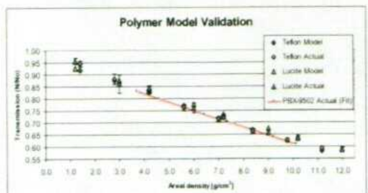


Fig. 4. Previous static radiograph taken of two polymer step wedges.



Plot 2. The calculated predictions match the radiograph data to within 3%. Transmission values include nuclear interactions. Between these two polymers, Teflon is a closer match to actual HE as represented by PBX-9502.

Step Wedges Built

1. 47.5% PET/ 52.5% PTFE → PBX-9501 Match
2. 44.5% PET/55.5% PTFE → PBX-9502 Match
3. PVDF → Average match for PBX-9501 & PBX-9501

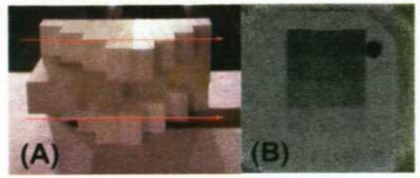
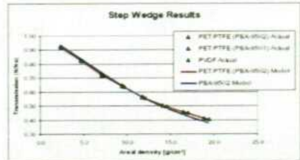
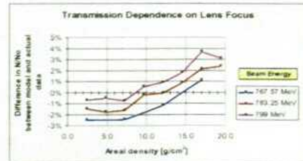


Fig. 5(A,B). Picture and radiograph of the stack of the step wedges. Beam direction is shown in red. PVDF is in-between the two PET/PTFE step wedges. The radiograph shows that the transmissions were very similar.



Plot 3. Data fit for the step wedges. Since the data points from the models are so similar, only the PET/PTFE (PBX-9502) Model was shown.



Plot 4. Changing the magnet settings for the lens system affects the beam energy and the transmission. These settings allow us to focus on different lengths of material.

Conclusions

The PET/PTFE polymer combinations turned out to be accurate simulants for both PBX-9501 and PBX-9502. These step wedges will aid in the analysis by making the use of HE calibrations unnecessary to calculate areal densities of HE in dynamic shots.

Material	Cost	Scaling factor	Accuracy to PBX-9501			Accuracy to PBX-9502		
			θ_o	dE/dx	N/No	θ_o	dE/dx	N/No
900-15 (PBX-9501 thermal mock)	>$5000	1.00	1.78%	2.32%	-0.11%	0.03%	-0.01%	0.00%
900-19 (PBX-9502 mock)	>$5000	1.16	0.89%	3.84%	-0.14%	-0.84%	1.48%	-0.03%
Cyanuric Acid	-	0.76	0.91%	2.78%	-0.12%	-0.82%	0.44%	-0.01%
Lucite® (PMMA)	~$200	1.70	0.71%	17.96%	-0.51%	-1.02%	15.27%	-0.39%
Teflon® (PTFE)	~$200	0.80	1.40%	-9.03%	0.29%	-0.34%	-11.10%	0.40%
Kynar® (PVDF)	~$200	1.04	0.81%	-2.03%	0.06%	-0.92%	-4.26%	0.17%
PET/PTFE: PBX-9501 match	~$400	1.04	0.03%	-0.10%	-0.05%	-1.69%	-2.37%	0.06%
PET/PTFE: PBX-9502 match	~$400	1.054	1.75%	2.36%	-0.15%	0.00%	0.03%	-0.03%

Table 2. Comparison of potential HE simulants. Values are from model predictions for materials that are scaled by length to match PBX-9501 and/or PBX-9502.

It is estimated that the areal densities calculated from a radiograph are within 3% of the actual values. However, the focal plane of the magnetic lens system and scattering from beam line "windows," and other sources of background are factors for error in calculations.

PVDF is proven to be a choice simulant for HE. As a single material without any scaling, it is within 0.3% of the transmission for the most common HE materials used in pRad.

Acknowledgements & References

Work presented here uses data and equations from:

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